Formyl chloride

2565-30-2 | DTXSID30180344

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.0549

Global applicability domain: Inside

Local applicability domain index: 4.22e-01

Confidence level: 5.65e-01

Nearest Neighbors from the Training Set

Image not found
Chloroacetonitrile
Measured: 0.45
Predicted: 4.54e-01

Image not found
1,4-Benzoquinone
Measured: 0.2
Predicted: 4.89e-01

Image not found
3-Chloropropionitrile
Measured: 0.18
Predicted: 3.72e-01

Image not found
Dimethyl sulfone
Measured: -1.41
Predicted: -1.07

Image not found
Thioglycolic acid
Measured: 0.09
Predicted: 1.90e-01